

Band filling effects on coherence lengths and penetration depth in the two-orbital negative- U Hubbard model of superconductivity

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Abstract

The two-orbital superconducting state is modeled by on-site intra-orbital negative- U Hubbard correlations together with inter-orbital pair-transfer interactions. The critical temperature is mainly governed by intra-orbital attractive interactions and it can pass through an additional maximum as a function of band filling. For the certain number of electrons the clear interband proximity effect is observable in the superconducting state of the band with a smaller gap. The influence of band fillings and orbital site energies on the temperature dependencies of two-component superconductivity coherence lengths and magnetic field penetration depth is analyzed. The presence of proximity effect is probably reflected in the relative temperature behaviour of characteristic lengths.

Keywords: two-orbital superconductor, coherence lengths, magnetic field penetration depth, Hubbard model, interband proximity effect

1. Introduction

The multi-component microscopic nature of superconductivity has been established in a number of materials (MgB₂ [1], cuprates [2], strontium rutenates [3], iron-arsenic compounds [4], Nb-doped SrTiO₃ [5], NbSe₂ [6], V₃Si [7] etc.). The first relevant theoretical scenarios have been discussed in the literature long time ago [8, 9, 10] and later on they have been developed for various systems (see e.g. Refs. [11, 12, 13, 14, 15] and references therein).

The peculiar properties of multi-component superconductors appear due to the involvement of coupled electron subsystems (orbitals, different Fermi surface sheets or other elements of electron structure) into the formation of superconducting ordering varying substantially the physical nature of the phenomenon and opening the possibilities for novel effects. As a result of the presence of inter-component pairing the certain quantities (e.g. coherence lengths and the relaxation times of superconductivity fluctuations) cannot be attributed to the initially independent subsystems and they describe the joint features of the whole two-component condensate [16, 17, 18, 19].

In a two-orbital superconductor with inter-orbital pairing, similarly to the results of Refs. [17, 20, 21], one of two solutions for coherence lengths diverges

near the phase transition point as a function of temperature, while the other one is non-critical [18]. We note also that the existence of critical and non-critical length scales in the coherency associates with the conception of critical and non-critical fluctuations [19, 22] in a two-component superconductor damping in different time-scales.

In the present contribution we continue to examine the temperature behaviour of characteristic lengths of a two-orbital superconductor described by negative- U Hubbard model [23] with inter-orbital pair-transfer interaction in dependence on the number of electrons. Our preliminary study has been done focusing on band filling effects in the spatial coherency including Van Hove singularity [18]. However, in that work [18] the orbital energy differences and charge fluctuations were neglected. In the present paper we clarify their role in the scaling of critical and non-critical coherence lengths and magnetic field penetration depth by band fillings. The numerical calculations have been carried out for a two-dimensional square lattice.

2. Superconductivity in a two-orbital system

Two-orbital superconductivity is modeled by the Hamiltonian of the following form (see e.g. [24]):

$$\begin{aligned}
H = & \sum_{\alpha} \sum_{i,j} \sum_{\sigma} [t_{ij}^{\alpha\alpha} + (\varepsilon_{\alpha}^0 - \mu) \delta_{ij}] a_{i\alpha\sigma}^{\dagger} a_{j\alpha\sigma} \\
& + \frac{1}{2} \sum_{\alpha} \sum_i \sum_{\sigma} U^{\alpha\alpha} n_{i\alpha\sigma} n_{i\alpha-\sigma} \\
& + \frac{1}{2} \sum_{\alpha,\alpha'} \sum_i \sum_{\sigma} U^{\alpha\alpha'} a_{i\alpha\sigma}^{\dagger} a_{i\alpha'\sigma}^{\dagger} a_{i\alpha-\sigma}^{\dagger} a_{i\alpha'-\sigma},
\end{aligned} \tag{1}$$

where $a_{i\alpha\sigma}^{\dagger}$ ($a_{i\alpha\sigma}$) is the electron creation (destruction) operator in the orbital $\alpha = 1, 2$ localized at the site i ; σ is the spin index; $t_{ij}^{\alpha\alpha}$ is the hopping integral; ε_{α}^0 is the orbital energy; μ is the chemical potential; $U^{\alpha\alpha} < 0$ is the intra-orbital attraction energy; $n_{i\alpha\sigma} = a_{i\alpha\sigma}^{\dagger} a_{i\alpha\sigma}$ is the particle number operator; $U^{\alpha\alpha'}$ with $\alpha \neq \alpha'$ is the inter-orbital interaction energy. Note that the both intra- and interorbital interaction channels involved lead to superconducting ordering.

In the reciprocal space the Hamiltonian (1) can be represented as

$$\begin{aligned}
H = & \sum_{\alpha} \sum_{\mathbf{k}} \sum_{\sigma} [\varepsilon_{\alpha}(\mathbf{k}) - \mu] a_{\alpha\mathbf{k}\sigma}^{\dagger} a_{\alpha\mathbf{k}\sigma} \\
& + \frac{1}{2N} \sum_{\alpha,\alpha'} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\mathbf{q}} \sum_{\sigma} U^{\alpha\alpha'} a_{\alpha\mathbf{k}\sigma}^{\dagger} a_{\alpha(-\mathbf{k}+\mathbf{q})-\sigma}^{\dagger} \\
& \times a_{\alpha'(-\mathbf{k}'+\mathbf{q})-\sigma} a_{\alpha'\mathbf{k}'\sigma}.
\end{aligned} \tag{2}$$

where $\varepsilon_{\alpha}(\mathbf{k})$ is the electron band energy associated with the orbital α and N is the number of lattice sites (number of atoms). The bulk superconducting state is described on the basis of the Hamiltonian (2) by means of the Hartree-Fock-Gorkov self-consistent equations

$$\begin{aligned}
\Delta_{\alpha} = & N^{-1} \sum_{\alpha'} U^{\alpha\alpha'} \sum_{\mathbf{k}} \langle a_{\alpha'-\mathbf{k}\downarrow} a_{\alpha'\mathbf{k}\uparrow} \rangle \\
= & \frac{-1}{N} \sum_{\alpha'} U^{\alpha\alpha'} \sum_{\mathbf{k}} \frac{\Delta_{\alpha}}{2E_{\alpha}(\mathbf{k})} \tanh \frac{E_{\alpha}(\mathbf{k})}{2k_B T},
\end{aligned} \tag{3}$$

$$\begin{aligned}
n_{\alpha} = & N^{-1} \sum_{\mathbf{k}} \sum_{\sigma} \langle a_{\alpha\mathbf{k}\sigma}^{\dagger} a_{\alpha\mathbf{k}\sigma} \rangle \\
= & \frac{1}{N} \sum_{\mathbf{k}} \left[1 - \frac{\tilde{\varepsilon}_{\alpha}(\mathbf{k})}{E_{\alpha}(\mathbf{k})} \tanh \frac{E_{\alpha}(\mathbf{k})}{2k_B T} \right],
\end{aligned} \tag{4}$$

$$\sum_{\alpha} n_{\alpha} = n. \tag{5}$$

Here $E_{\alpha}(\mathbf{k}) = \sqrt{\tilde{\varepsilon}_{\alpha}^2(\mathbf{k}) + |\Delta_{\alpha}|^2}$, $\tilde{\varepsilon}_{\alpha}(\mathbf{k}) = \varepsilon_{\alpha}(\mathbf{k}) + \frac{1}{2} U^{\alpha\alpha} n_{\alpha} - \mu$, n_{α} are the occupation numbers of orbitals

(bands) per lattice site, and n is the total number of electrons per site. The Eqs. (3) determine the superconducting gaps of orbitals (bands), the Eq. (4) gives us the orbital occupation numbers and the Eq. (5), the chemical potential μ in dependence on n and other relevant quantities. The temperature of superconducting phase transition T_c satisfies the equation

$$\begin{vmatrix} 1 + U^{11} g_1(T_c) & U^{12} g_2(T_c) \\ U^{21} g_1(T_c) & 1 + U^{22} g_2(T_c) \end{vmatrix} = 0, \tag{6}$$

where

$$g_{\alpha}(T) = \frac{1}{2N} \sum_{\mathbf{k}} \frac{1}{\tilde{\varepsilon}_{\alpha}(\mathbf{k})} \tanh \frac{\tilde{\varepsilon}_{\alpha}(\mathbf{k})}{2k_B T}. \tag{7}$$

In the general case of spatial inhomogeneity and non-zero magnetic field we have the following Ginzburg-Landau equations

$$\begin{aligned}
\Delta_{\alpha}(\mathbf{r}) = & - \sum_{\alpha'} U^{\alpha\alpha'} \left[g_{\alpha'}(T) - \nu_{\alpha'} |\Delta_{\alpha'}(\mathbf{r})|^2 \right. \\
& \left. + \beta_{\alpha'} \left(\nabla + i \frac{2\pi}{\Phi_0} \mathbf{A} \right)^2 \right] \Delta_{\alpha'}(\mathbf{r}).
\end{aligned} \tag{8}$$

$$\begin{aligned}
\mathbf{j}_s = & -i \frac{2\pi}{V_0 \Phi_0} \sum_{\alpha} \beta_{\alpha} \{ \Delta_{\alpha}^*(\mathbf{r}) \nabla \Delta_{\alpha}(\mathbf{r}) \\
& - \Delta_{\alpha}(\mathbf{r}) \nabla \Delta_{\alpha}^*(\mathbf{r}) \} \\
& - \frac{2}{V_0} \left(\frac{2\pi}{\Phi_0} \right)^2 \left(\sum_{\alpha} \beta_{\alpha} |\Delta_{\alpha}(\mathbf{r})|^2 \right) \mathbf{A}.
\end{aligned} \tag{9}$$

Here

$$\begin{aligned}
\nu_{\alpha} = & \frac{-1}{2N} \sum_{\mathbf{k}} \frac{\partial}{\partial |\Delta_{\alpha}|^2} \left[\frac{1}{E_{\alpha}(\mathbf{k})} \right. \\
& \times \left. \tanh \frac{E_{\alpha}(\mathbf{k})}{2k_B T_c} \right]_{\Delta_{\alpha}=0},
\end{aligned} \tag{10}$$

$$\beta_{\alpha} = \beta_{\alpha 1} = \beta_{\alpha 2} = \beta_{\alpha 3} \tag{11}$$

with

$$\begin{aligned}
\beta_{\alpha l} = & \frac{-1}{4N} \sum_{\mathbf{k}} \frac{\partial^2}{\partial q_l^2} \left\{ \frac{1}{\tilde{\varepsilon}_{\alpha}(\mathbf{k}) + \tilde{\varepsilon}_{\alpha}(\mathbf{k} - \mathbf{q})} \right. \\
& \times \left[\tanh \left(\frac{\tilde{\varepsilon}_{\alpha}(\mathbf{k})}{2k_B T_c} \right) \right. \\
& \left. \left. + \tanh \left(\frac{\tilde{\varepsilon}_{\alpha}(\mathbf{k} - \mathbf{q})}{2k_B T_c} \right) \right] \right\}_{\mathbf{q}=0},
\end{aligned} \tag{12}$$

\mathbf{A} is the vector potential, \mathbf{j}_s is the density of supercurrent, Φ_0 is the magnetic flux quantum and V_0 is the volume of unit cell. According to the Eq. (11) we restrict ourselves to the isotropic electron energy spectrum.

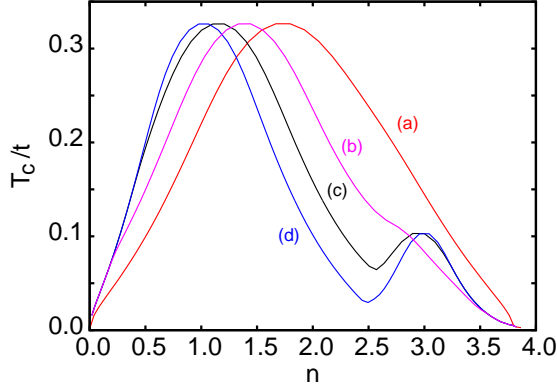


Figure 1: The critical temperature T_c versus band filling $n = n_1 + n_2$ for various $\varepsilon_1^0/t = 0, 1, 2, 3$, curves (a)–(d), respectively.

3. Characteristic lengths of a two-orbital superconductor

By considering the solutions of Eqs. (8) which correspond to the small deviations of gaps from their bulk values, $\eta_\alpha(\mathbf{r}) = \Delta_\alpha(\mathbf{r}) - \Delta_\alpha$, one can find two length scales characterizing the spatial behaviour of superconductivity in a two-orbital system:

$$\xi_{s,r}^2(T) = \frac{G(T) \pm \sqrt{G^2(T) - 4K(T)\gamma}}{2K(T)}, \quad (13)$$

where

$$\begin{aligned} G(T) &= (U^{12})^2 [\tilde{g}_1(T)\beta_2 + \tilde{g}_2(T)\beta_1] \\ &- [1 + U^{11}\tilde{g}_1(T)]U^{22}\beta_2 \\ &- [1 + U^{22}\tilde{g}_2(T)]U^{11}\beta_1, \end{aligned} \quad (14)$$

$$\begin{aligned} K(T) &= [1 + U^{11}\tilde{g}_1(T)][1 + U^{22}\tilde{g}_2(T)] \\ &- (U^{12})^2 \tilde{g}_1(T)\tilde{g}_2(T) \end{aligned} \quad (15)$$

with $\tilde{g}_\alpha(T) = g_\alpha(T) - 3\nu_\alpha(\Delta_\alpha(T))^2$, and

$$\gamma = [U^{11}U^{22} - (U^{12})^2]\beta_1\beta_2. \quad (16)$$

The soft or critical coherence length $\xi_s(T)$ diverges at the phase transition point $T = T_c$, while the rigid or non-critical coherence length $\xi_r(T)$ remains finite.

On the basis of Eq. (9) one obtains in a standard way the magnetic field penetration depth for a two-orbital superconductor,

$$\lambda = \sqrt{\frac{V_0\Phi_0^2}{8\pi^2\mu_0 \sum_\alpha \beta_\alpha |\Delta_\alpha|^2}}, \quad (17)$$

where μ_0 is the magnetic permeability of free space.

4. Numerical results

Below we present the results of numerical calculations for two-dimensional square lattice with hopping integrals between nearest neighbours $t_{ij}^{\alpha\alpha} = t$ and electron band energies associated with s -orbitals $\varepsilon_\alpha(\mathbf{k}) = \varepsilon_\alpha^0 - 2t[\cos(ak_x) + \cos(ak_y)]$, a is the lattice constant, and $-\frac{\pi}{a} \leq k_{x,y} \leq \frac{\pi}{a}$. The intra- and interorbital interactions are chosen as $U^{11} = -1.5t$, $U^{22} = -2.5t$, $|U^{12}| = |U^{21}| = 0.04t$, and the site energy ε_2 is fixed at $\varepsilon_2^0 = 0$. In all calculations we have chosen $k_B = 1$.

Using Eqs. (6) and (7) we calculated the superconducting critical temperature T_c . Fig. 1 shows the dependence of T_c on the band filling $n = n_1 + n_2$. One can see that the curve T_c vs n is most symmetric as $\varepsilon_1^0 = \varepsilon_2^0$ (see Fig1, curve (a)). In this case, the small shift of the maximum of T_c towards the smaller values of occupation number n is caused by effective Hartree corrections $U^{\alpha\alpha}n_\alpha/2$. First of all, these corrections are different for various orbitals as the intra-orbital interactions $U^{\alpha\alpha}$ are different. Consequently, the distances between the chemical potential μ position and the lower edges of orbital bands are slightly different. Therefore the position of the maximum of T_c is moved reflecting the above mentioned difference which appears here due to the choice of intra-orbital pairing potentials $|U^{22}| > |U^{11}|$.

By increasing the difference between the bare site energies $|\varepsilon_1^0 - \varepsilon_2^0|$ we observe that the asymmetry of the function $T_c(n)$ increases. In the cases (a) and (b) in Fig. 1, the site energies of orbitals are closer and the influence of the Hartree terms does not lead to dramatically different distances between the chemical potential and lower band edges. As a result the single peak in T_c vs n is preserved. However, with the further increase of the difference between of bare site energies $\varepsilon_{1,2}^0$ the effect of the Hartree renormalization $|\varepsilon_1^0 + U^{11}n_1/2 - \varepsilon_2^0 - U^{22}n_2/2|$ becomes stronger and we observe the splitting of the single peak of T_c into two maxima (see Fig1, curves (c) and (d)) caused by the circumstance that the chemical potential passes in the region $0 \leq n \leq 4$ two Van Hove singularities related to the bands $\alpha = 1, 2$. It should be also noted that the larger values of $|\varepsilon_1^0 - \varepsilon_2^0|$ mean the larger difference between the band occupation numbers n_1 and n_2 which corresponds to the stronger Hartree renormalization.

Next we solve the gap equations (Eq. (3)) below T_c . In Fig. 2 one can see the plotted superconducting gaps Δ_α vs temperature for different band fillings. Note that the increase of n changes the order of Δ_1 and Δ_2 in the energy scale for fixed temperature, c.f. Figs. 2a, 2b and 2c, 2d. With that for the intermediate values on n

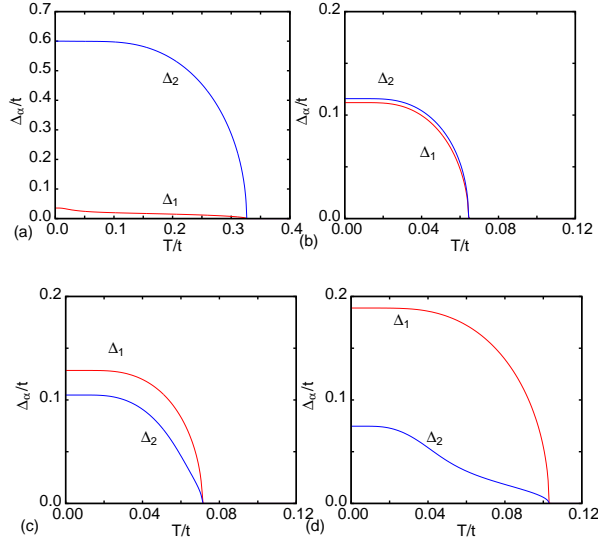


Figure 2: The temperature dependence of superconducting gaps for fixed $\varepsilon_1^0/t = 2$ and $n = 1.10, 2.57, 2.64, 2.90$, panels (a)–(d), respectively.

the gaps Δ_1 and Δ_2 are relatively close (Figs. 2b and 2c) while for $n = 1.1$ and $n = 2.9$ one of the gaps strongly dominates (Figs. 2a and 2d). The latter peculiarity is caused by the chemical potential vicinity to the Van Hove singularity which supports superconductivity in the corresponding band. The weaker superconductivity in another band is related, at least partially, to the interband proximity effect. At the same time the band fillings $n = 1.1$ and $n = 2.9$ correspond approximately to the maxima of $T_c(n)$ in Fig. 1. Thus, the formation of two peaks of T_c as a function of n in Fig. 1 reflects the redistribution of the driving roles of bands in the appearance of superconductivity.

In a single-orbital (single-band) system the Ginzburg-Landau parameter $\kappa = \lambda/\xi$ defines the type-I ($\kappa < 1/\sqrt{2}$) and type-II ($\kappa > 1/\sqrt{2}$) superconductivity. The coherence lengths (see Eq. (13)) and magnetic field penetration depth (see Eq. (17)) for two-orbital model are plotted in Fig. 3 for the band fillings discussed above. Apart from the divergence of the soft length scale ξ_s at T_c , we observe also a maximum for the rigid length scale ξ_r slightly below T_c in Figs. 3b and 3c. This is due to the closeness of the superconductivity gaps for these band fillings, see Figs. 2b and 2c.

Another interesting observation is related to the crossing point of ξ_r and λ . In Figs. 3b–d this cross-

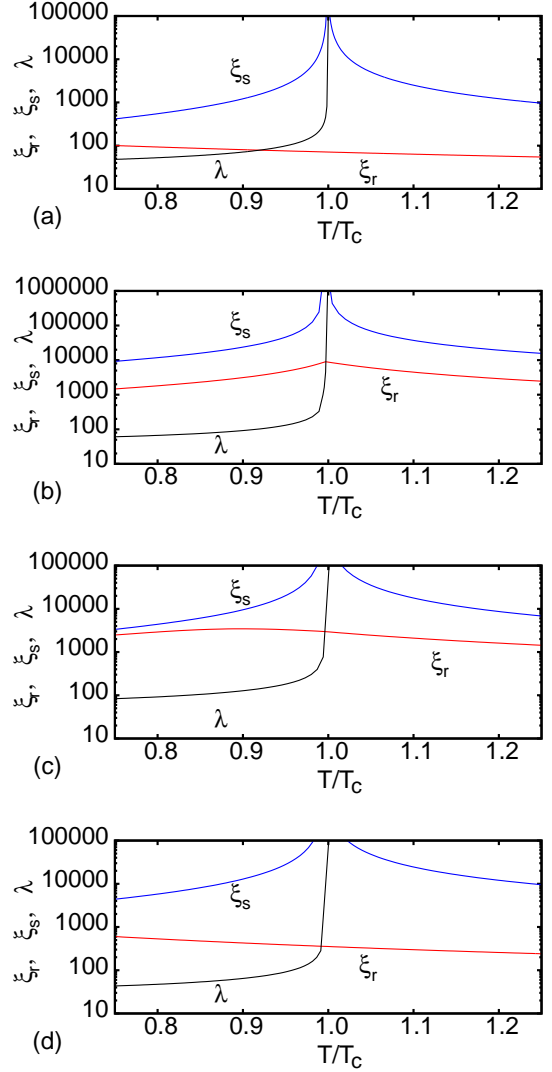


Figure 3: The temperature dependence of coherence lengths and magnetic field penetration depth in units of the lattice space a for fixed $\varepsilon_1^0/t = 2$ and $n = 1.10, 2.57, 2.64, 2.90$, panels (a)–(d), respectively.

ing appears at the temperatures very close to T_c while in Fig. 3a the crossing point is located remarkably lower in the temperature scale. Thus, there exists always a small temperature region in Figs 3a–d where $\xi_r < \lambda < \xi_s$ ¹. One can treat the fulfilment of the inequality $\xi_r < \sqrt{2}\lambda < \xi_s$ as necessary but not sufficient

¹We have used the relatively small values of attractive interaction $|U^{aa}|$ to make the Hartree-Fock-Gorkov approximation plausible. In this situation we found that the penetration depth in our calculations is always smaller than the critical coherence length. The negative-U Hubbard model for larger $|U^{aa}|$ has to be treated in a different way [23].

condition for type-1.5 superconductivity [26], see Ref. [16]. To shed more light on the problem one has to study the character of the interaction between vortices [16].

The larger extent of the temperature region in Fig. 3a where $\xi_r < \lambda < \xi_s$ may be related to the interband proximity effect which is more pronounced in this case (see Fig. 2a). It was shown in [27] that type-1.5 superconductivity can arise due to the proximity effect in a two-band system.

5. Conclusions

We presented the results of band filling effect on two-orbital superconductor. The dependencies of critical and non-critical coherence lengths on temperature were compared to the penetration depth for different electron numbers. It was shown that the band structure including site energy and position of Van Hove singularity is important for superconducting gaps temperature behaviour as well as in the relationship between the magnitudes of critical and non-critical coherence lengths and penetration depth. We have identified a temperature region where $\xi_r < \lambda < \xi_s$. Its larger extent could be associated with the presence of interband proximity effect in a two-orbital superconducting system.

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